Development of Cell/Pack Level Models for Automotive Li-Ion Batteries with Experimental Validation

Chao-Yang Wang (PI)

Christian Shaffer (Presenter)

EC Power

http://www.ecpowergroup.com

6/17/14

Project ID #
ES120

Overview

Timeline

- Start date: 5/1/2011
- End date: 4/30/2014
- Project 97% complete

Barriers

- Barriers addressed
  - LiB Performance and Lifetime
  - LiB Efficiency
  - LiB Safety
  - Computer tools for design exploration

Budget

- Total project funding: $3.0M
  - $1.5M (DOE)
  - $1.5M (cost share)
  - Fed funds received to date: $1.276M

Partners

- Ford
- Johnson Controls
- Penn State
- NREL
- ORNL

Funding provided by **Dave Howell** of the DOE Vehicle Technologies Program .
The activity is managed by **Brian Cunningham** of Vehicle Technologies.
Subcontracted by NREL, **Shriram Santhanagopalan** Technical Monitor

Project Objectives - Relevance

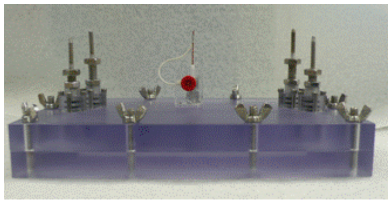
- Develop an electrochemical/thermal (ECT) coupled model for large-format automotive Li-ion batteries (cells and packs)
- Create a fast & robust tool for realistic geometries
- Develop a comprehensive materials database
- Integrate ECT3D software with CAEBAT Open Architecture Standard (OAS)
- Aide OEMs and cell/pack developers in accelerating the adoption of large-format Li-ion technology required for EV & PHEV
- Develop a virtual environment to reduce the time required for design, build and test of Li-ion batteries
  - Performance
  - Safety
  - Life
  - Efficiency
- Support DOE CAEBAT activity

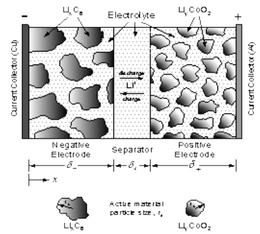
Project Milestones & Activities

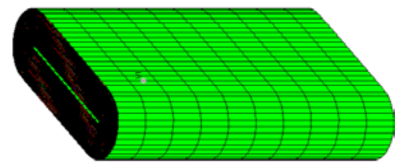
Recent Milestones Completed
M17: Deliver updated software to partners with OAS compatibility
M18: Complete data of electrode potential curves for series of aged cells
M22: Additional data for LFP cathode and LTO anode
M23: Report on experimental data for exchange current density
M24: Report on current and temperature validation
M26 & 27: Report on life model validation
M29: Report on 3-electrode cell experiments for performance and life

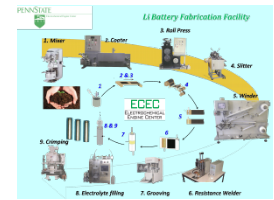
Milestones in Progress
M25: Final report on software
M28: Deliver final software to partners
M30: Final report on temperature distribution data
M31: Final report on OAS compatibility
M32: Final project report

Approach – Supporting CAEBAT Activity









Task 1: Materials Characterization (PSU)

Task 2: Physico-chemical Models (ECP)

Task 3: Advanced Algorithms (ECP)

Task 4: Experimental Validation (PSU, ECP)

EC Power software: ECT3D

Ford, JCI

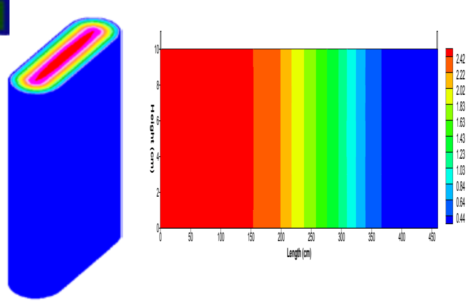
Feedback

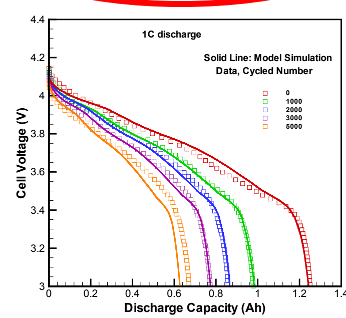
Feedback

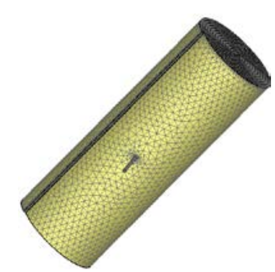
Performance

Cycle Life

Safety

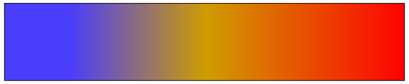






Approach – Materials Database

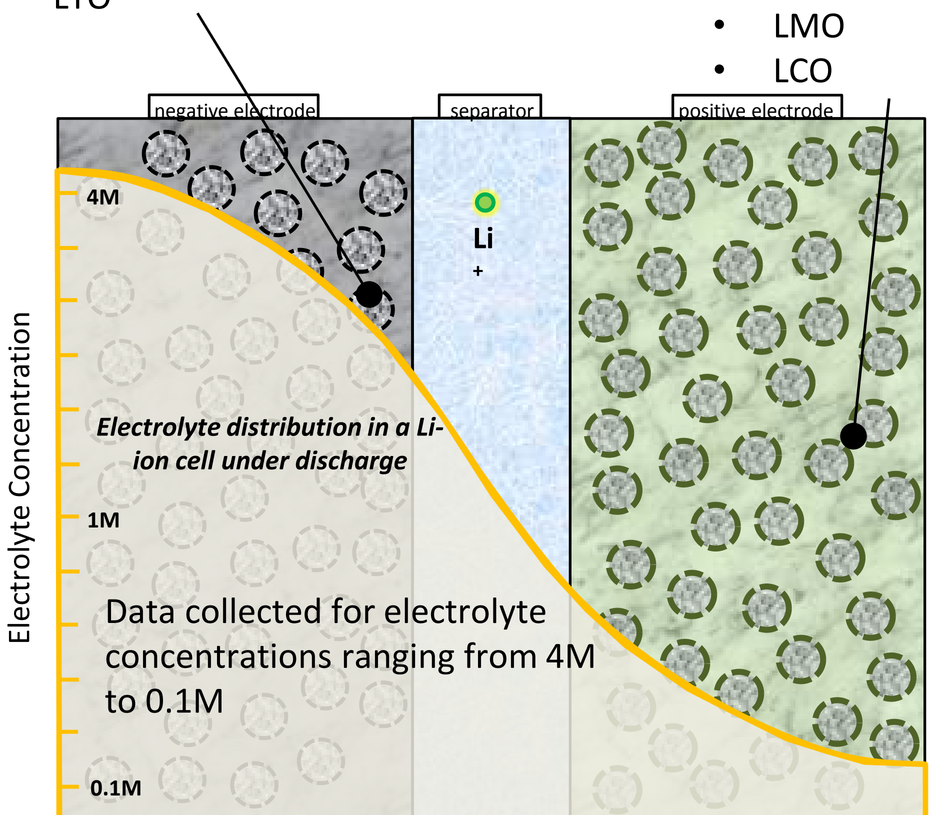
Tested temperature range for materials



-30°C **100°C**

Anode Materials:
- Graphite (blended natural/synthetic)
- LTO

Cathode materials:
- NCM
- LFP
- LMO
- LCO



Data collected for electrolyte concentrations ranging from 4M to 0.1M

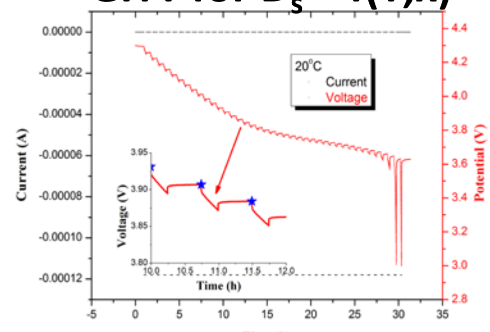
- Database data acquisition complete
  - Active cathode and anode materials given to the left
  - Electrolyte

Thousands

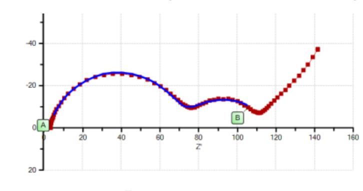
of coin cells

- Massive undertaking spanning length of project
- High quality material properties lead to validated results for large format cells and packs

GITT for $D_s = f(T,x)$



EIS for $i_o = f(T,x,c_e)$



Modeling parameters needed at ***low-T, high-T, wide range of chemical compositions*** and similar conditions of interest for ***automotive Li-ion batteries and packs***.

Approach – ECT Model Development

Electrochemical Processes
- electrochemical reactions
- solid state diffusion
- ion transport through electrolyte
- charge transfer

Heat generation rate

$$q = \sum_j a_{sj} \bar{i}_{nj} \left(\bar{\eta}_j + \Pi_j \right) - \sum_k \left[< \mathbf{i}_k > \cdot \nabla < \phi_k >^k \right]$$

Thermal Processes

- conservation of thermal energy

$$\frac{\partial \left(\rho c_p T \right)}{\partial t} = \nabla \cdot \boldsymbol{\lambda} \nabla T + q$$

Temperature-dependent physico-chemical properties

$$\Phi = \Phi_{ref} \exp\left[\frac{E_{act,\Phi}}{R} \left(\frac{1}{T_{ref}} - \frac{1}{T} \right) \right]$$

Model predictions
- potential and current curves
- temperature history/distribution
- active material utilization
- current distribution

- Understanding thermal phenomena & thermal control has huge impact on
  - Battery safety
  - Cycle life
  - Battery management system
  - Cost

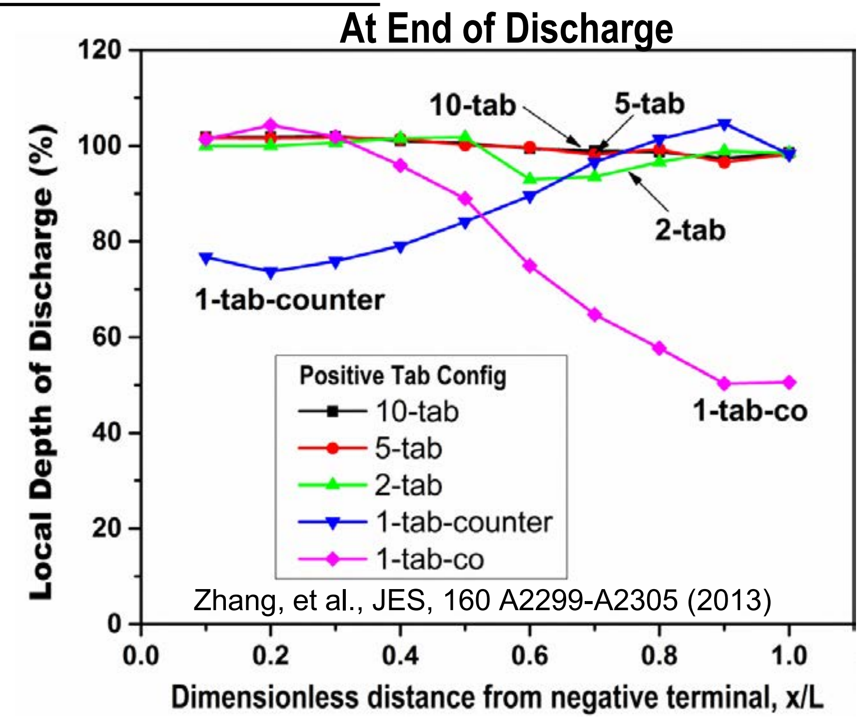
- Electrochemical-thermal (ECT) coupling required for
  - Safety simulations
  - Thermal runaway
  - High power, low-T operation
  - Heating from subzero environment

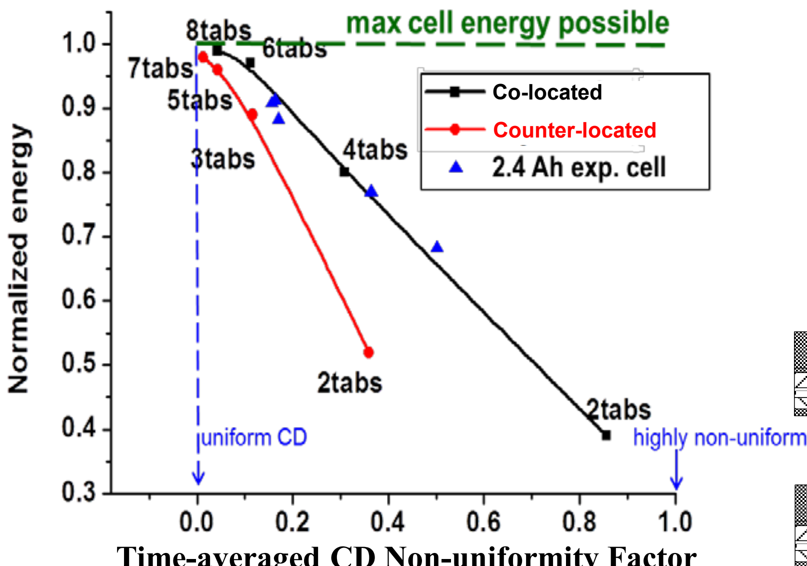
Technical Accomplishments

- Completed data acquisition for materials database
- Validated efficient, electrochemical-thermal (ECT) coupled large-format cell simulation
  - Performance and active materials utilization
- Validated temperature- and design-dependent life model
  - LFP/graphite and NMC/graphite
  - User-defined load profile and thermal conditions
- Validated safety model
- ECT-coupled pack model
- Demonstrated co-simulation with OAS
- Software commercially available

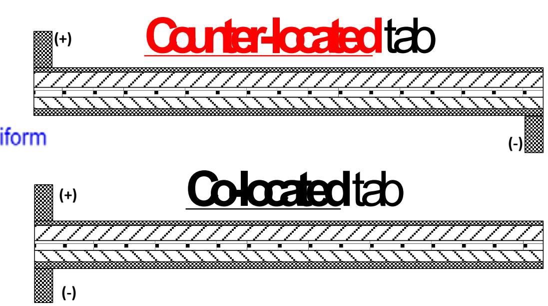
Accomplishments – Validation/Performance

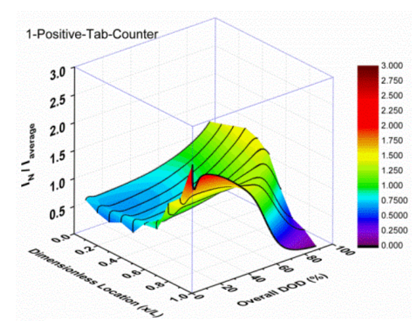
In-situ Current Distribution





W. Zhao et al. J. Power Sources 257 70-79 (2014)





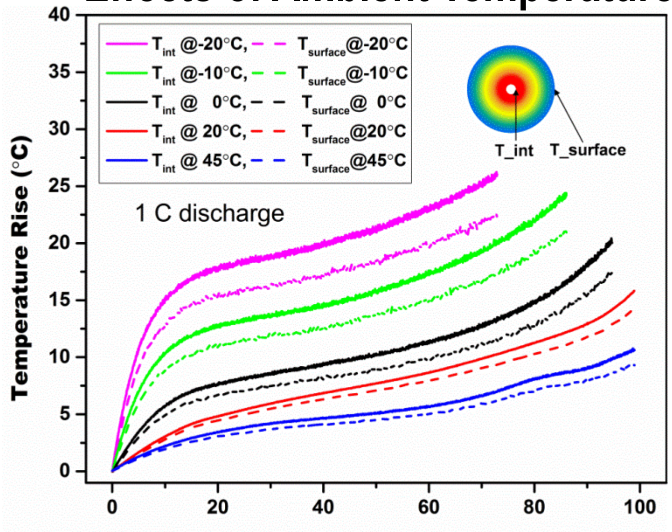
1-positive-tab-counter

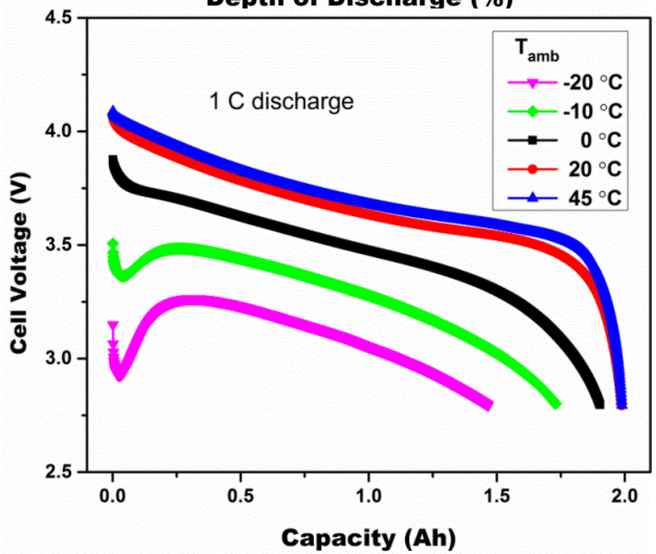
***Direct measurement and validation** of **in-situ current density** of a large-format Li-ion battery; ensuring current uniformity is critical for **utilization of active material,** directly **effecting energy density** (up to 50%)*

Accomplishments – Validation/Performance

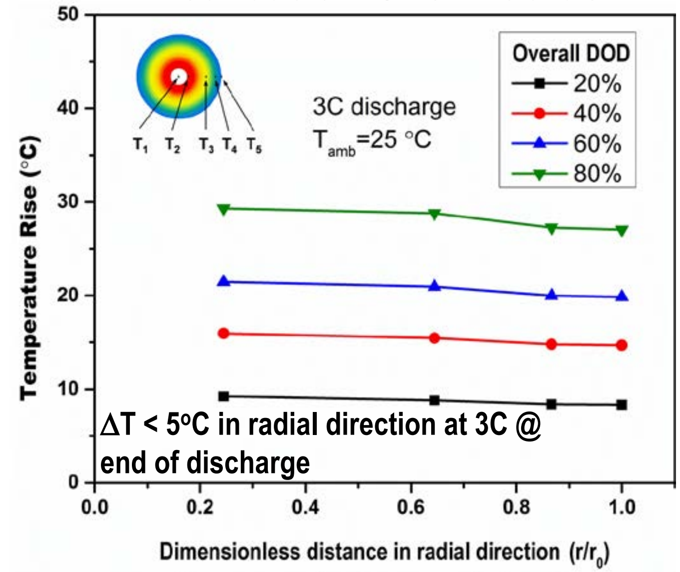
In-situ Temperature Distribution

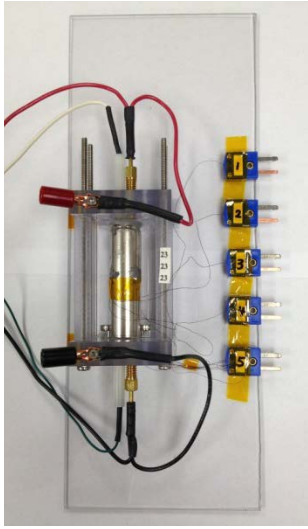
Effects of Ambient Temperature





Distribution Over Radius





- In-situ temperature measurement within Li-ion battery
- Data acquired over wide-ranging temperature, C-rate, and thermal boundary conditions
- Validation ongoing

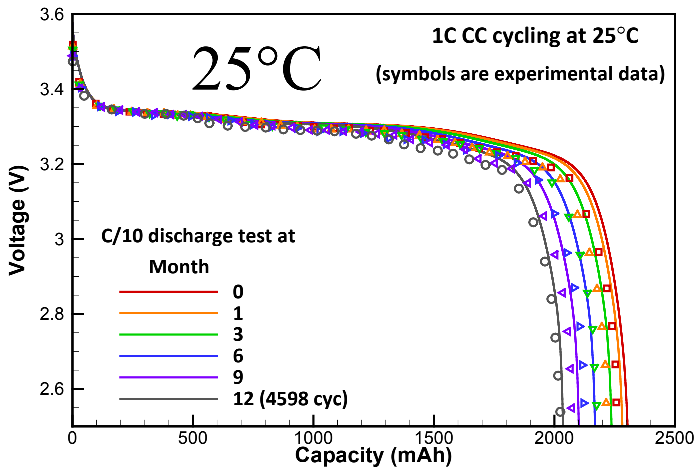
Direct measurement and validation of in-situ temperature distribution

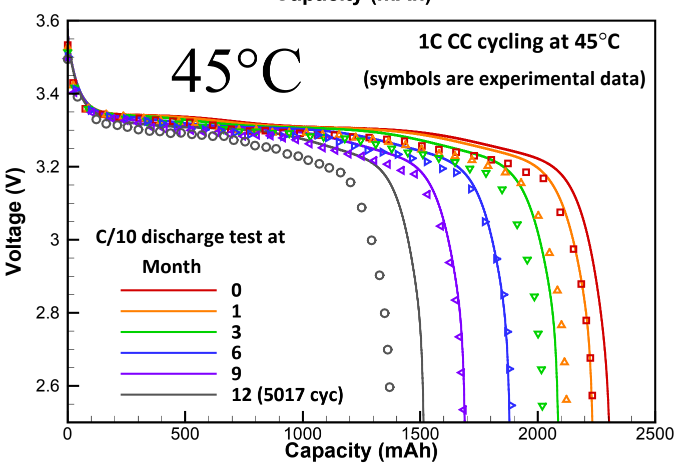
Accomplishments – Validation/Life

EC POWER

Commercial LFP/Graphite Cells

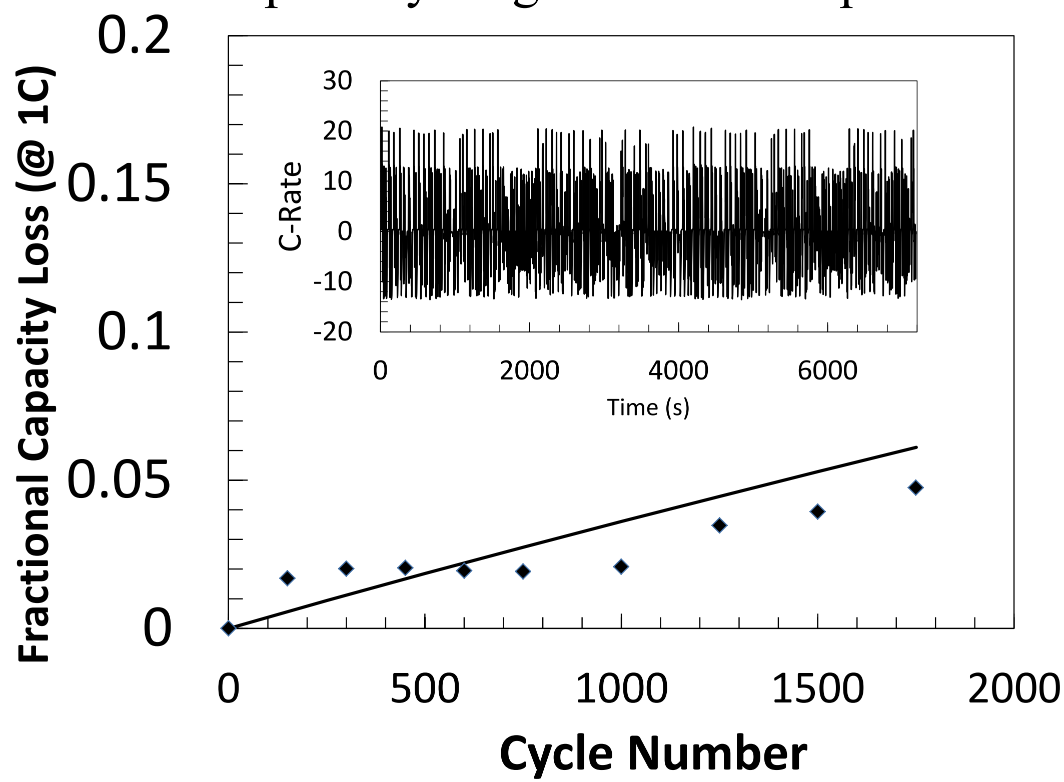
CC Cycling @ 25^{o}C and 45^{o}C





A123 ANR26650M1-B: Graphite-LFP high power cell
Data from Safari & Delacourt, *JES*, 258(5) A562, 2011

Complex Cycling at Room Temperature

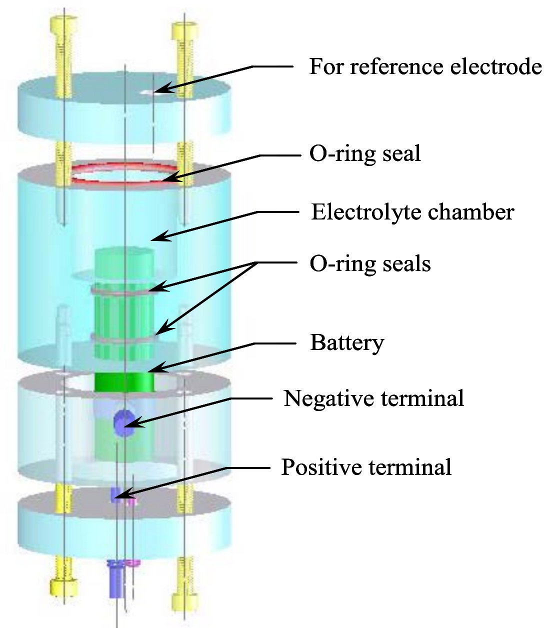


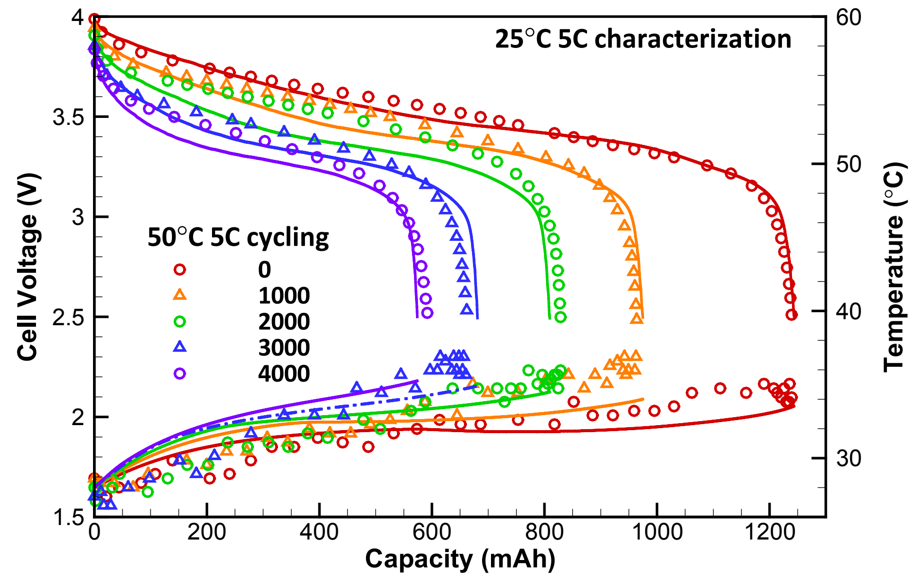
- On-field relevant cycling at 25°C
- Commercial LFP/graphite cell
- Internal life data

<u>On-field relevant life cycling</u> *of* ***commercial Li-ion cells*** *successfully captured with model at* ***different temperatures;*** *all life models are* ***mechanism-based*** *and valid under wide operating conditions without calibration*

Accomplishments –Validation/Life

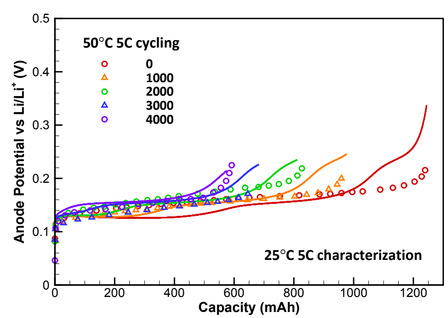
NMC/Graphite Cells



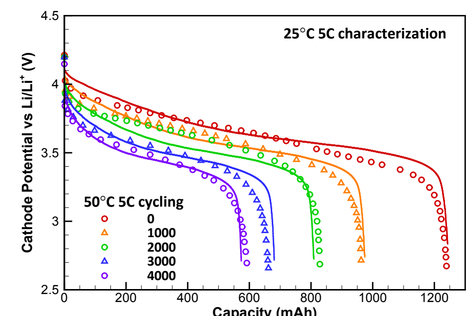


Full cell characterization at 5C, 25°C

- CC cycling at 50°C, 5C-rate
- NMC/graphite cell
- In-house data obtained using 3-electrode cell
- Use of individual electrode potentials for more rigorous validation of life mechanisms in models



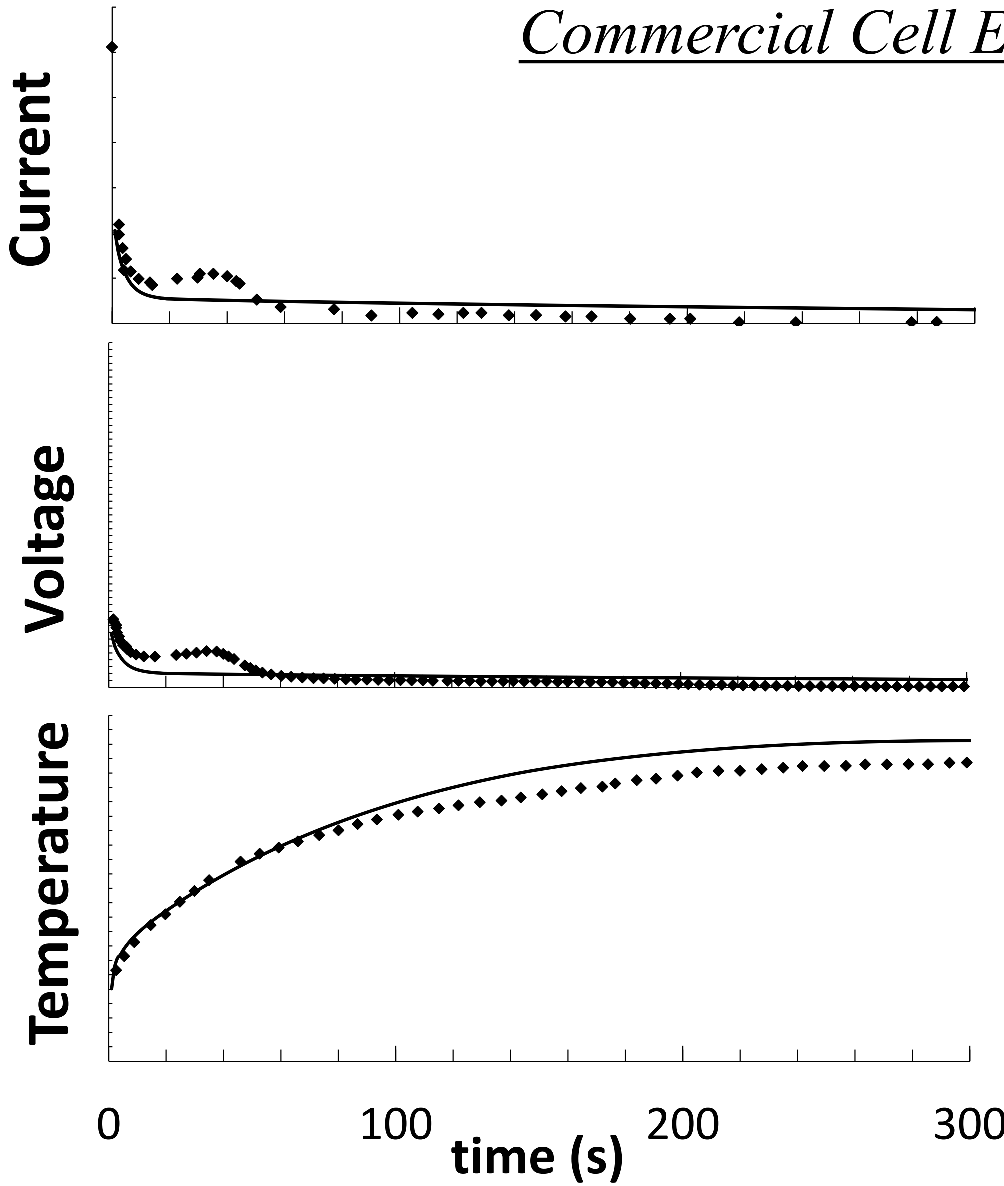
Anode at 5C



Cathode at 5C

***Degradation mechanisms** in **each electrode** validated using 3-electrode cell*

Accomplishments – Safety/Validation

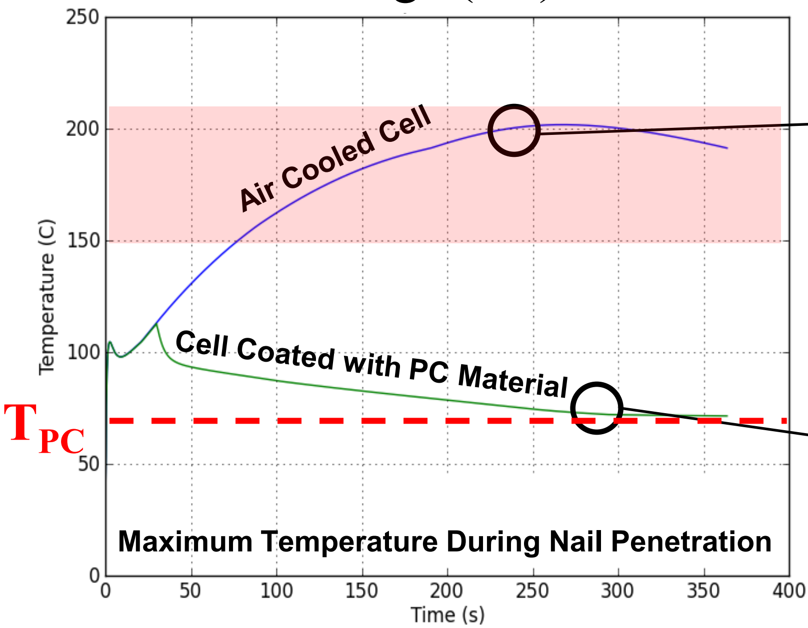


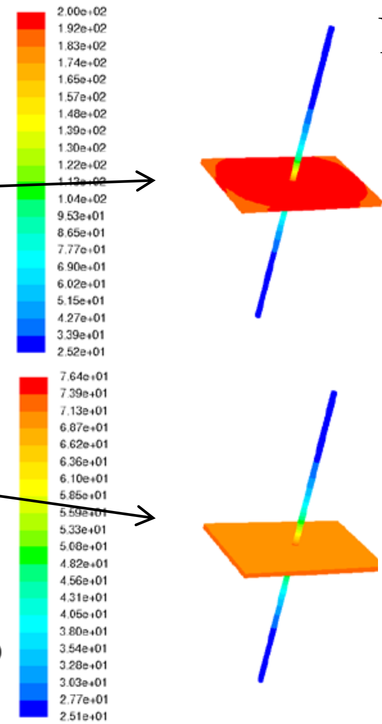
- External short of one cell within commercial pack
- Dimensionless current, voltage, and temperature data shown on the left
- Good agreement between data and simulation (temperature within ~ 10%)
- Maximum temperature reached during shorting process can be used to assess safety of design

*Software developed can be used to **assess the safety of commercial large-format batteries***

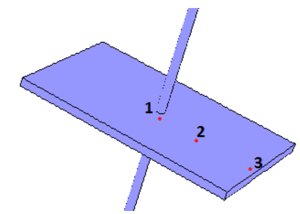
Safety Simulations in ECT3D

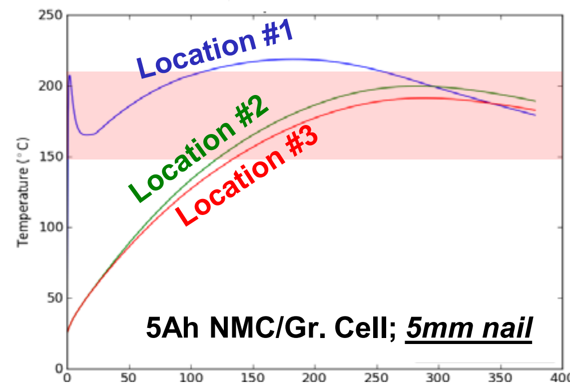
Nail Penetration with Coated Phase-change (PC) Material

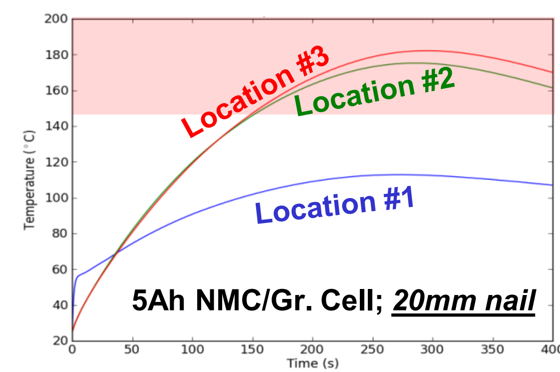




Physics of Shorting During Nail Penetration







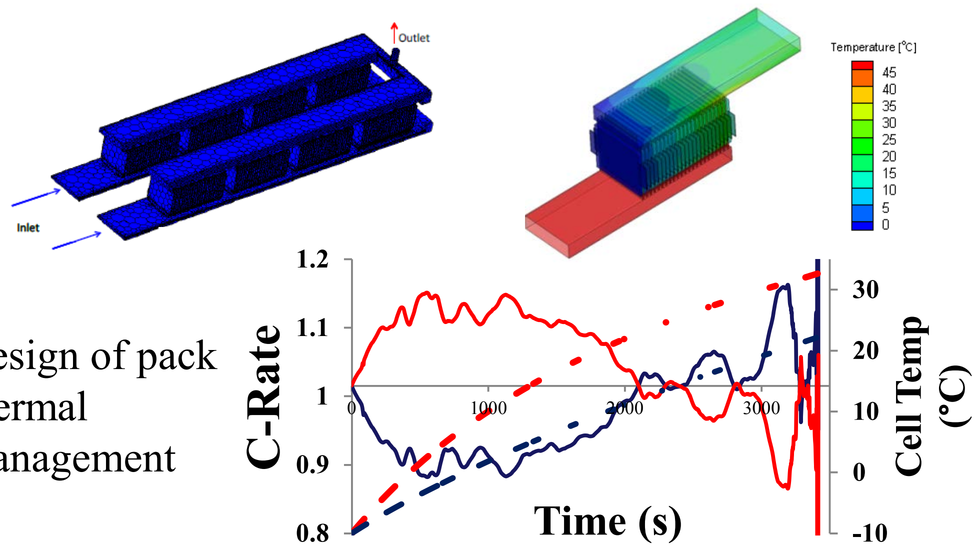
- Software gives coupled electrochemical-thermal response of the cells during nail penetration events
- Time scale and locality of heating dictate ability of safety designs to maintain cell safety
  - 5mm nail: short time scale, local heating
  - 20mm nail: long time scale global heating

*ECT3D is used routinely for **safety evaluation of large-format cells and safety-conscious designs***

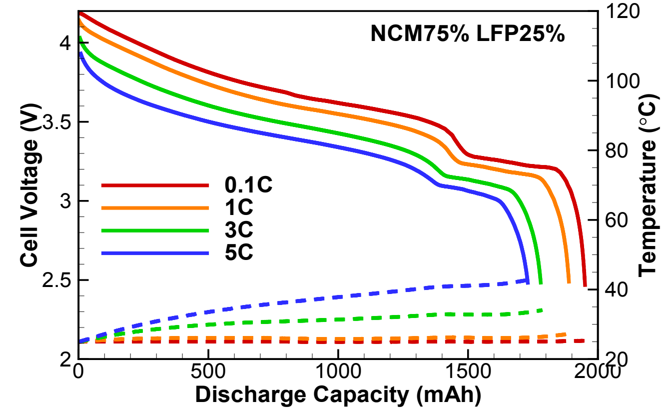
Accomplishments – Other

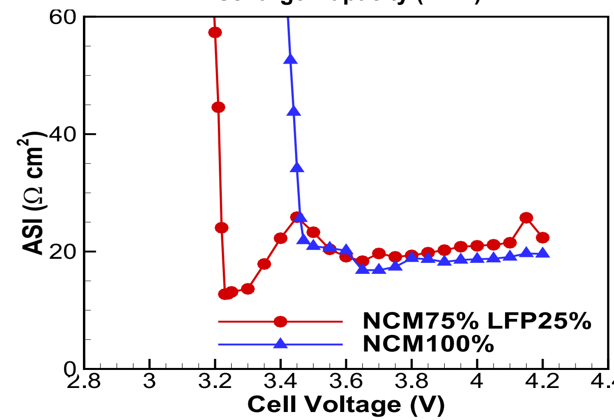
Thermally-coupled Pack Modeling

Design of pack thermal management



Mixed Electrode Model



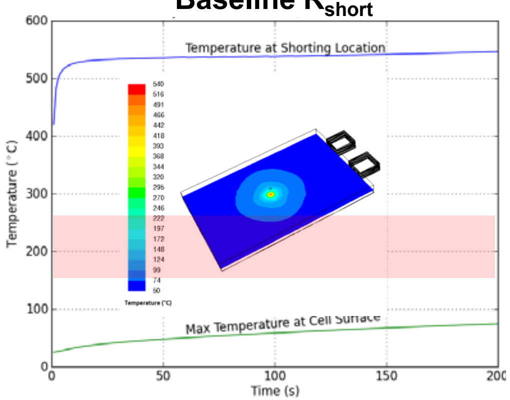


Similar results shown in literature: Gallagher et al. JPS 196 (2011) 9702-9707

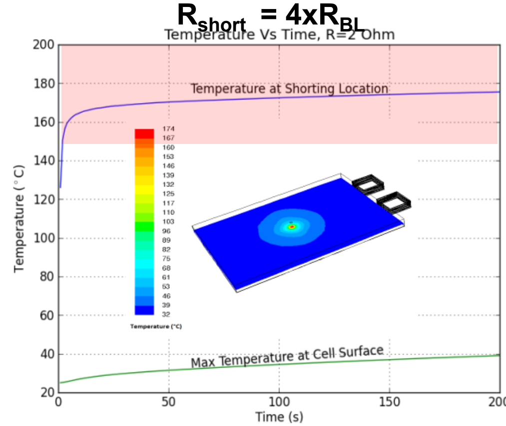
- Above example shows mixed electrode model used to improve low SOC power via blended NMC/LFP mixture

Cell Internal Shorting

Baseline R_{short}



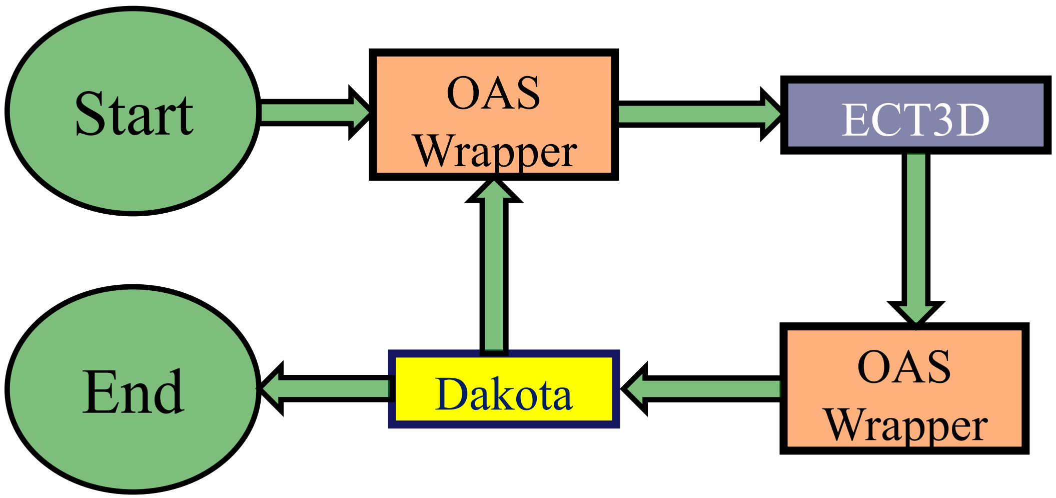
$R_{short} = 4xR_{BL}$



Other routine uses of software: ***pack thermal management*** *design,* ***safety evaluation of large-format cells and safety-conscious designs,*** *and* ***designing batteries with optimal power and energy tradeoff***

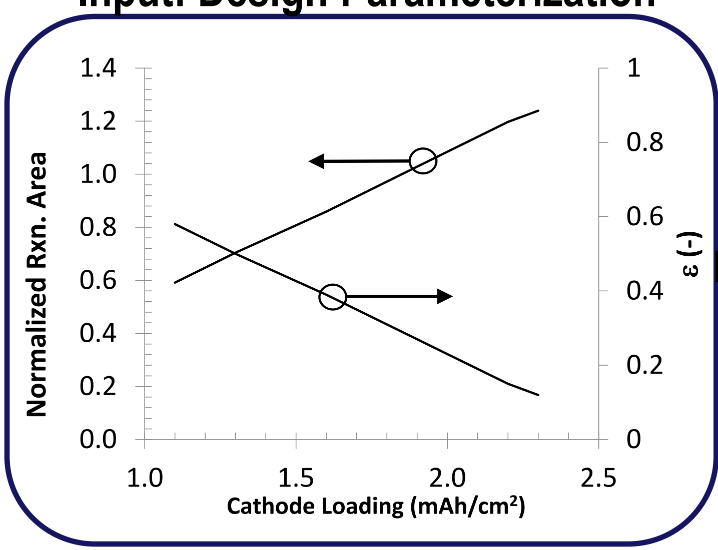
Accomplishments – OAS

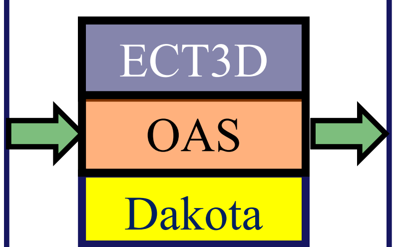
ECT3D Coupled to Dakota Using OAS



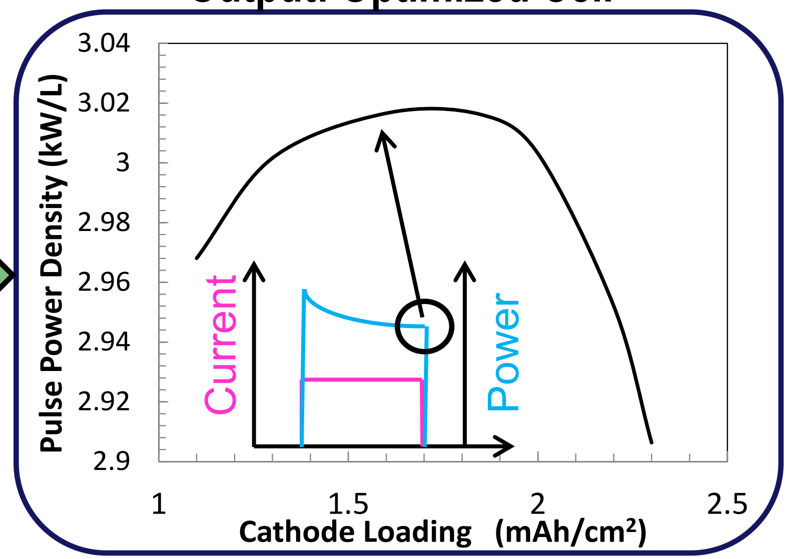
- ECT3D successfully coupled to Dakota optimization software via OAS
- Design optimization demonstrated below
- ECT3D can be coupled to other softwares (e.g. industry internal or other 3rd party) via OAS

Input: Design Parameterization





Output: Optimized Cell



ECT3D has been successfully coupled to other software via OAS

Accomplishments – Publications

- Wei Zhao, C.Y. Wang, Gang Luo, Christian E. Shaffer, "New Findings on Large Li-ion Battery Safety through Computer Simulation", Battery Safety 2011- Advancements in System Design, Integration, & Testing for Safety & Reliability, **November 9-10, 2011**, Las Vegas, NV
- G. Luo and C.Y. Wang, A Multi-dimensional, Electrochemical-Thermal Coupled Li-ion Battery Model, Chap.6 in Lithium-Ion Batteries: Advanced Materials and Technologies, CRC Press, **2012**.
- Yang, Xiao Guang, Miller, Ted and Yu, Paul, Ford Motor Company, "Li-Ion Electrochemical Model," 2012 Automotive Simulation World Congress, **October 30-31, 2012**, Detroit, MI
- Shaffer, C.E., Wang, C.Y., Luo, G. and Zhao, W., "Safety Analysis Design of Lithium-ion Battery EV Pack through Computer Simulation," Battery Safety 2012, Knowledge Foundation Conference, **December 6-7, 2012**, Las Vegas, NV
- Shaffer, C.E. and Wang, C.Y., "Thermal Management for Start-up of Li-Ion Batteries," 222nd Meeting of The Electrochemical Society (PRiME 2012), Honolulu, HI, **October 7-12, 2012**
- Luo, Gang, Shaffer, C.E. and Wang C.Y., "Electrochemical-thermal Coupled Modeling for Battery Pack Design," 222nd Meeting of The Electrochemical Society (PRiME 2012), Honolulu, HI, **October 7-12, 2012**
- Kalupson, J., Luo, G. and Shaffer, C., "AutoLion™: A Thermally Coupled Simulation Tool for Automotive Li-ion Batteries," SAE Technical Paper 2013-01-1522, 2013, doi: 10.4271/2013-01-1522. SAE International World Congress and Exhibition, **April 16, 2013**, Detroit, MI
- Ji, Y., Zhang, Y., and Wang, C.Y. (**2013**). "Li-Ion operation at low temperatures," Journal of the Electrochemical Society, 160(4), A636-A649
- Zhang, G., Shaffer, C. E., Wang, C. Y., & Rahn, C. D. (**2013**). "In-situ measurement of current distribution in a li-ion cell," Journal of the Electrochemical Society, 160(4), A610-A615
- Ji, Y., Wang, C.Y. (**2013**). "Heating strategies for Li-ion batteries operated from subzero temperatures," Electrochimica Acta, 107, 664-674
- Guangsheng Zhang, Christian E. Shaffer, Chao-Yang Wang, and Christopher D. Rahn, "Effects of Non-uniform Current Distribution on Energy Density of Li-ion Cells," Journal of the Electrochemical Society, 160 A2299-A2305 (**2013**)
- G.S. Zhang, L. Cao, S. Ge, C.Y. Wang, C. E. Shaffer, C. D. Rahn, In Situ Measurement of Li-Ion Battery Internal Temperature, 224th ECS Meeting, Abstract #538, San Francisco, CA, USA, Oct. 27 - Nov. 01, **2013**
- W. Zhao, G. Luo, and C.Y. Wang, "Effect of Tab Design on Large-format Li-ion Cell Performance," Journal of Power Sources 257 70-79 (**2014**)
- G.S. Zhang, L. Cao, S. Ge, C.Y. Wang, C. E. Shaffer, C. D. Rahn, "In Situ Measurement of Temperature Distribution in a Cylindrical Li-ion Cell," to be submitted (**2014**)
- W. Zhao, G. Luo and CY Wang, "Modeling Nail Penetration Process in Large-Format Li-ion Cells," submitted to J power sources (**2014**)

Collaboration w/Other Institutions

Funding Agency

CAEBAT Program Administrator

Open Architecture Software

Project Lead – Software development and sales, project administration.

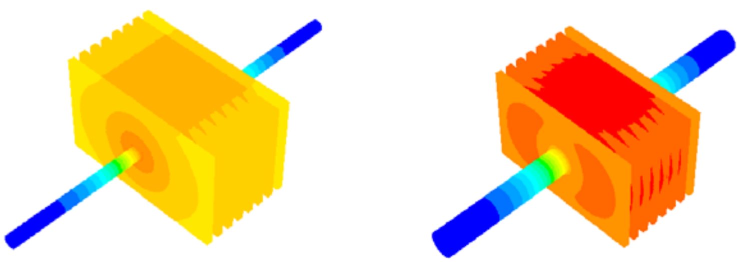
Industrial Partner – testing, validation, and feedback

Industrial Partner – testing, validation, and feedback

Academic Partner – materials testing and detailed model validation

Future Work

- Wrap up final deliverables for this project
  - M25: Final report on software
  - M28: Deliver final software to partners
  - M30: Final report on temperature distribution data
  - M31: Final report on OAS compatibility
  - M32: Final project report
- Outside of this project
  - Pack-level safety
  - Abuse simulation
  - Refined life models



Response to Previous Year Review

- Last year's review did not include an individual presentation from our team (CAEBAT overall project presentation/review was given by NREL)

Summary

- All main project goals have been met
  - Development of ECT-coupled cell and pack model
  - Materials database for commercially relevant materials, accurate over wide-ranging T, c_e, SOC, etc.
  - Validated prediction of performance and active material utilization
  - Validated safety models
  - Validated life models
- Commercial partners (Ford, JCI)
  - Have been using updated models in-house for several years
  - Have given invaluable feedback and helped validate model
- Software is commercially available
- Meeting CAEBAT/DOE goals
  - Helping to accelerate the adoption of automotive Li-ion battery cells & packs
  - Enabling technology for EV, PHEV